TNF target flame: Premixed H_2/air and NH_3/H_2/air flames in turbulent boundary layers

Authors

Cheng Chi[a], Benedicte Cuenot[b], Dominique Thévenin[a]

Affiliations

[a] Laboratory of Fluid Dynamics and Technical Flows, Otto von Guericke University Magdeburg, D-39106, Germany

[b] CERFACS, 42 avenue Gaspard Coriolis, Toulouse, 31047, France

Introduction

Direct numerical simulations (DNS) of turbulent head-on quenching of premixed H_2/air and NH_3/H_2/air flames in fully developed turbulent channel flows at friction Reynolds number $\mathrm{Re}_\tau \approx 300$ were conducted. Both adiabatic and isothermal walls were considered. Both the unity-Lewis number approach and detailed molecular transport model have been tested. There are several objectives of these DNS simulations: (i) to check the near-wall flame dynamics and combustion regime variations [1]; (ii) to check the effect of differential diffusion on quenching characteristics [2]; (iii) to check the pollutant emission characteristics for the near-wall flames [3], and (iv) to examine the near-wall flame marker [4]. The dataset includes more than 10 snapshots from the initiation of the flame to complete flame quenching for each flame configuration. All thermochemical and flow variables are stored.

DNS configuration and methods

The DNS were preformed using our in-house low-Mach combustion solver DINO [5]. The detailed NH_3 mechanism [6] and H_2 mechanism [7] were applied for the NH_3/H_2/air and H_2/air flames, respectively. For molecular transport, both the mixture-averaged diffusion model [8] and unity-Lewis number approach were tested. The thermodiffusion (Soret) effect was not considered. The governing equations were solved spatially using a 6th order centered finite difference method and temporally using a 4th order Runge-Kutta explicit method. Chemical reactions are solved by Cantera [9].

Operation conditions

Non-reacting channel flows are firstly simulated until the wall turbulence is fully developed. The channel has streamwise (x), wall-normal (y) and spanwise (z) lengths of $5h$, $2h$ and $2h$, respectively, where h = 5 mm is the half-width of the channel. Afterwards, two identical flame fronts (mapped from 1D unstretched freely propagating flame solutions) are initiated at $y = 0.5h$ and $y = 1.5h$, with burned gases in the channel center and flames propagating towards the top and bottom cold walls. More numerical details are listed in Table 1.

Table 1: Numerical details of all the DNS cases. u_τ is the friction velocity, $l^* = \nu/u_\tau$ is the viscous length scale, ν is the kinematic viscosity, $\mathrm{Re}_\tau = hu_\tau/\nu$ is the friction Reynolds number, $\mathrm{Da}_w = t_w/t_L$ is the wall Damköhler number, $t_w = \nu/u_\tau^2$ and $t_L = \delta_L/S_L$ are the wall and flame time scales respectively, S_L and δ_L are the laminar flame speed and thickness respectively, α is the fuel H_2 volume ratio, ϕ is the mixture equivalence ratio, T_u and T_w are the unburned and wall temperatures respectively, ISO represents isothermal wall, while AD represents adiabatic wall, MA represents mixture-averaged diffusion model, while UL represents unity Lewis number approach.

	Case HIM	Case AIM	Case HAM	Case AAM	Case HIU	Case AIU
u_τ (m/s)	6.40	5.13	6.40	5.13	6.40	5.13
l^* (μm)	17.86	15.97	17.86	15.97	17.86	15.97
Re_τ	280	313	280	313	280	313
Da_w	0.167	0.004	0.167	0.004	0.167	0.004
α	1.0	0.2	1.0	0.2	1.0	0.2
ϕ	1.5	1.0	1.5	1.0	1.5	1.0
T_u (K)	750	750	750	750	750	750
T_w (K)	ISO 750	ISO 750	AD	AD	ISO 750	ISO 750
S_L (m/s)	14.54	0.843	14.54	0.843	14.54	0.843
δ_L (mm)	0.243	0.661	0.243	0.661	0.243	0.661
t_w (μs)	2.79	3.11	2.79	3.11	2.79	3.11
t_L (μs)	16.7	784	16.7	784	16.7	784
MDM	MA	MA	MA	MA	UL	UL

The hydrogen flames are simulated with a grid resolution $\Delta x^+ = 2.71$ (uniformly 48.4 μm), $\Delta z^+ = 2.189$ (uniformly 39.1 μm), and $0.437 \leq \Delta y^+ \leq 1.635$ (stretched grids in the wall-normal direction from 7.8-29.2 μm). The ammonia/hydrogen flames are simulated with a grid resolution $\Delta x^+ = 2.023$ (uniformly 32.3 μm), $\Delta z^+ = 2.448$ (uniformly 39.1 μm), and $0.326 \leq \Delta y^+ \leq 1.215$ (stretched grids in the wall-normal direction from 5.2-19.4 μm).

Exemplary results

Figure 1 shows the propagation of the flames in the channel flow.

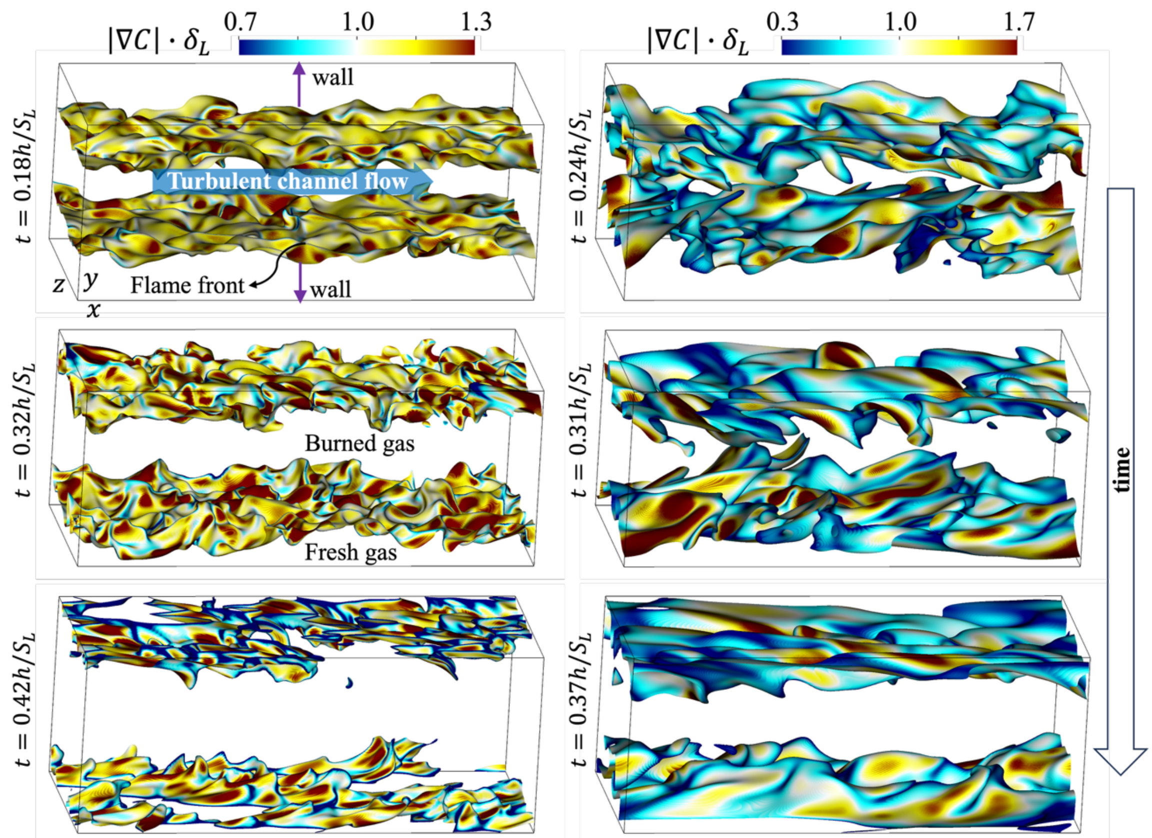

Figure 1: Propagation of the flame surfaces for the H_2/air flame (left, Case HIM) and NH_3/H_2/air flame (right, Case AIM). The flame surface is indicated by $C = 0.55$ in Case HIM and $C = 0.78$ in Case AIM, with progress variable C defined by Y_{H2O}.

How to get access to the data

Upon request. Contact Cheng Chi (cheng.chi@ovgu.de)

A single snapshot can be found on Zenodo: https://doi.org/10.5281/zenodo.14025205

References

[1] C. Chi, B. Cuenot, D. Thévenin, Turbulent flame-wall interaction: dynamics of flame thickness and combustion regime, J. Fluid Mech. 1029 (2026) A5.

[2] C. Chi, C. Yu, B. Cuenot, U. Maas, D. Thévenin, Effect of differential diffusion on head-on quenching of premixed NH3/H2/air flames within turbulent boundary layers, Proc. Combust. Inst. 40 (2024) 105276.

[3] C. Chi, Flame dynamic insights into emission characteristics of NH3/H2/air combustion in turbulent boundary layers, Combust. Flame 269 (2024) 113723.

[4] C. Chen, C. Chi, W. Han, L. Yang, D. Thévenin, A flame marker for ammonia/hydrogen/air premixed flames during flame/wall interactions, Proc. Combust. Inst. 41 (2025) 105935.

[5] A. Abdelsamie, G. Fru, T. Oster, F. Dietzsch, G. Janiga, D. Thévenin, Towards direct numerical simulations of low-Mach number turbulent reacting and two-phase flows using immersed boundaries, Comput. Fluids 131 (2016) 123–141.

[6] Y. Jiang, A. Gruber, K. Seshadri, F. Williams, An updated short chemical-kinetic nitrogen mechanism for carbon-free combustion applications, Int. J. Energy Res. 44 (2) (2020) 795–810.

[7] J. Li, Z. Zhao, A. Kazakov, F.L. Dryer, An updated comprehensive kinetic model of hydrogen combustion, Int. J. Chem. Kinet. 36 (10) (2004) 566–575.

[8] J.O. Hirschfelder, C.F. Curtiss, R.B. Bird, The molecular theory of gases and liquids, John Wiley & Sons, 1964.

[9] D.G. Goodwin, H.K. Moffat, I. Schoegl, R.L. Speth, B.W. Weber. Cantera: An object-oriented software toolkit for chemical kinetics, thermodynamics, and transport processes. https://www.cantera.org, 2025. Version 3.2.0.